Micro- and Macrostates in the Einstein Crystals

In this project we will address the micro- and macro-states of an Einstein crystal. You will learn how to represent and count microstates in a simple model of a crystal consisting of a set of independent oscillators, you will learn how to find the probability of a macrostate for two Einstein crystals in thermal contact, and to find the time evolution of the Einstein crystal using a Monte Carlo simulation technique.

A simple model for a crystal that still captures surprisingly many of the important features of the statistical physics of a crystal is the Einstein crystal. A real crystal consists of a set of atoms in a periodic configurations interacting through interatomic interactions that include both short range and longer ranged forces. As a result, individual atoms will oscillate around an equilibrium position while interacting mostly with its nearest neighbors. As a simplified model for this system we consider each atom, i, to behave like an independent harmonic oscillator with a potential energy U_i:

$$U_i(\vec{r}_i) = \frac{1}{2}k_x(x_i - x_{i,eq})^2 + \frac{1}{2}k_y(y_i - y_{i,eq})^2 + \frac{1}{2}k_z(z_i - z_{i,eq})^2 \ ,$$

From quantum mechanics, we know that the energy of a harmoic oscillator i is

$$\epsilon_i = n_i \Delta \epsilon \ ,$$

where n_i is an integer describing the state of oscillator i. We can therefore describe the state of a crystal with N independent (meaning non-interacting) oscillators by the states n_i for $i = 1, \ldots, N$. The total energy of the crystal in this simplified model is then:

$$U = \sum_{i=1}^{N} \epsilon\, n_i \ .$$

For simplicity we will measure energy in units of ϵ:

$$q = \frac{U}{\epsilon} = \sum_{i=1}^{N} n_i \ ,$$

For a system with a given total energy, the sum of all the n_i is constant, but we can still change how the energy is distributed in the system. We can think of the energy a given number of energy units that we are free to distribute between the oscillators. Any distribution is allowed as long as we do not change the total energy.

We describe a microstate of this system by the numbers n_i for each oscillator:

$$\{n_1, n_2, \ldots, n_N\}$$

For example, for a system with $N = 4$ and $q = 4$, a possible microstate is $\{1, 0, 2, 1\}$, that is $n_1 = 1$, $n_2 = 0$, $n_3 = 2$, and $n_4 = 1$.

We will now find the various microstates of this system:

(a) For a system with $N = 2$ oscillators and $q = 3$, list all the possible microstates.

Solution:
The sum of the energy of the permissible microstates is $q = 2$. We therefore have two units of energy that we can distribute between two oscillators. This can be done in the following ways:

$\{2,0\}$
$\{1,1\}$
$\{0,2\}$

(b) For a system with $N = 3$ oscillators and $q = 3$, list all the possible microstates.

Solution:
The sum of the energy of the permissible microstates is $q = 3$. We therefore have three units of energy that we can distribute between three oscillators. This can be done in the following ways:

$\{3,0,0\}$
$\{0,3,0\}$
$\{0,0,3\}$
$\{2,1,0\}$
$\{2,0,1\}$
$\{0,2,1\}$
$\{1,2,0\}$
$\{0,1,2\}$
$\{1,0,2\}$
$\{1,1,1\}$

The general formula for the number of microstates for N oscillators with q units of energy is:

$$\Omega(N, q) = \left(\begin{array}{c} q + N - 1 \\ q \end{array} \right) = \frac{(q + N - 1)!}{q!(N - 1)!} .$$

(c) Check that the results you found above are consistent with this formula.

We can now list and count the number of microstates for an Einstein crystal, and we are ready to address what happens if two Einstein crystals come in contact. First, we start by looking at a system consisting of two isolated Einstein crystals, system A with N_A oscillators and energy q_A and system B with N_B oscillators and energy q_B. Each system is surrounded by an insulating, rigid and impermeable outer wall so that its energy, volume and number of oscillators (particles) is constant. The total system consists of system A and system B, so that $N = N_A + N_B$ and $q = q_A + q_B$. However, the systems are initially isolated – meaning that they are independent systems with constant energy, volume and number of particles.

(d) For a system consisting of subsystem A with $N_A = 2$ and $q_A = 5$ and subsystem B with $N_B = 2$ and $q_B = 1$ list all possible microstates of the system.

Solution:
For each microstate in system A there are two possible microstates in system B, all energy in oscillator b_1 or all energy in oscillator b_2. We therefore only list the microstates of system A

a_1	a_2	b_1	b_2
5	0	1	0
4	1	1	0
3	2	1	0
2	3	1	0
1	4	1	0
0	5	1	0
5	0	0	1
4	1	0	1
3	2	0	1
2	3	0	1
1	4	0	1
0	5	0	1

The two systems are put in thermal contact, so that they can exchange energy, but the number of particles and the volume of each subsystem does not change. The total energy $q = q_A + q_B = 6$ is constant, but the energy can now be freely distributed between the two systems. Let us now count the number of possible microstates for each possible value of q_A and q_B.

(e) For $N_A = 2$, $N_B = 2$, and $q = 6$ what are the possible values of q_A and q_B? We call a state with a given q_A (and therefore also a given $q_B = q - q_A$) a macrostate for the system.

Solution:
We know that $q = q_A + q_B = 6$, hence $q_A = 0, 1, 2, 3, 4, 5, 6$ and $q_B = q - q_A = 6 - q_A$.

(f) For each possible macrostate q_A find the number of compatible microstates.

Solution:
For each of the possible macrostates q_A we use the formula

$$\Omega = \Omega_A(N_A, q_A)\Omega_B(N_B, q_B)$$

to find the number of microstates. This is done in the following program:

```
% Calculate  number  of  microstates  for  two
%      Einstein - crystals  in  contact
NA  =  2;
NB  =  2;
q  =  6;
multA  =  zeros(q,1);
multB  =  multA;
mult  =  multA;
N  =  NA  +  NB;
qvalue  =  (0:q);
for  ik  =  1:length(qvalue)
  qA  =  qvalue(ik);
  qB  =  q  -  qA;
  multA(ik)  =  nchoosek(qA+NA-1,qA);
  multB(ik)  =  nchoosek(qB+NB-1,qB);
  mult(ik)  =  multA(ik)*multB(ik);
end
summult  =  sum(mult);
prob  =  mult./summult;
plot(qvalue,prob)
arr  =  [qvalue'  multA  multB  mult]
arr2  =  [qvalue'  prob]
```

The output is:

q_A	Ω_A	Ω_B	$\Omega_A\Omega_B$
0	1	7	7
1	2	6	12
2	3	5	15
3	4	4	16
4	5	3	15
5	6	2	12
6	7	1	7

(g) Compare the total number of microstates available to the system before and after the systems came in thermal contact. Comment on the result. What aspects of this result do you think is general?

Solution:
Before: Number of microstates is $\Omega_A(N_A, q_A)\Omega_B(N_A, q_B)$ for given values of q_A and q_B.

After: Number of microstates is $\Omega = \sum_{q_A} \Omega_A(N_A, q_A)\Omega_B(N_B, q_B)$.

General: More states after than before.

(h) If all microstates have the same probability, what are the probability of each of the macrostates?

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q_A	$P(q_A)$
0	0.0833
1.0000	0.1429
2.0000	0.1786
3.0000	0.1905
4.0000	0.1786
5.0000	0.1429
6.0000	0.0833

(i) What is the probability of the initial macrostate before the two systems came in contact?

Solution:
This corresponds to $q_A = 5$, and the prob is 0.1429.

(j) What is the probability of finding all the energy in system A?

Solution:
This corresponds to $q_A = 6$, $P = 0.0833$.

(k) What is the probability of finding exactly half the energy in system A?

Solution:
Half the energy is $q_A = 3$, prob $P = 0.1905$. The maximal value.

We will now address larger systems numerically. You therefore need to write a script/program to find the number of macrostates and the probability of the macrostates. We start from the system we had above, but you will need to write a general program you can use for any value of N_A, N_B, q, and q_A.

(l) For $N_A = N_B = 2$ and $q = 6$ write a program to find the number of microstates for each macrostate q_A and the probability $P(q_A) = \Omega(N_A, q_A)\Omega(N_B, q_B)/\Omega_{TOT}$ for each macrostate. Compare with your results from above. Plot the probabilty $P(q_A)$ as a function of q_A.

Solution:
The program is listed above.

We will now address a larger system with $N_A = 50$, $N_B = 50$ and $q = q_A + q_B = 100$.

(m) Plot the probability $P(q_A)$ as a function of q_A for all possible values of q_A.

Solution:
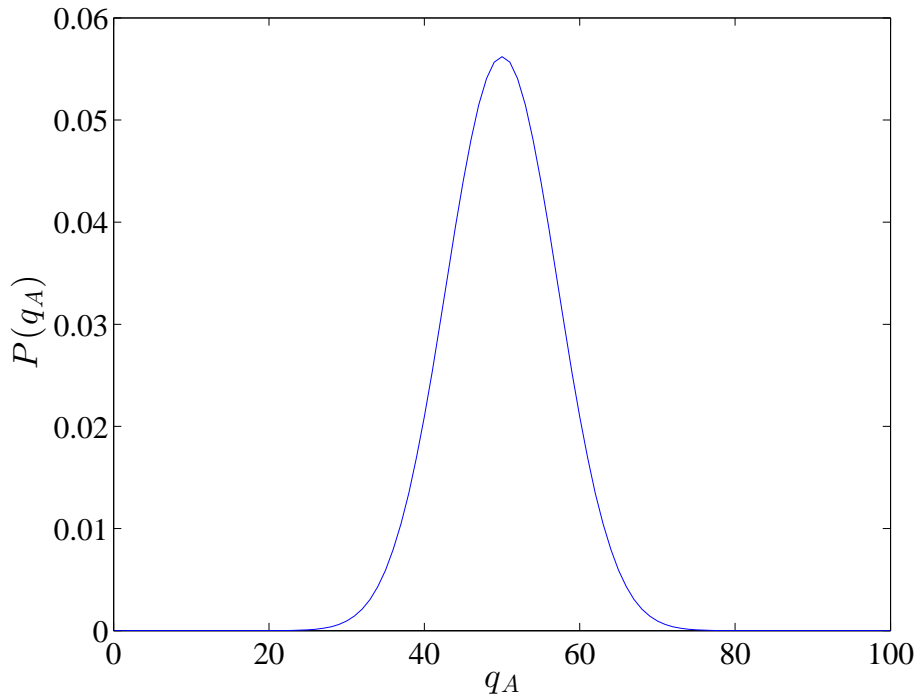The program is listed above.

Figure 1: Plot of the probability $P(q_A)$ for $N_A = N_B = 50$ and $q = 100$.

(n) What is the most probable macrostate? What is the probability of the system being in the most probable macrostate compared to all other macrostates in the system? Comment on the result.

Solution:
The most probable macrostate occurs for $q_A/N_A = q_B/N_B = q/N$, that is for $q_A = 50$. The probability for this macrostate is 0.0562.

(o) We start from a system with $q_A = 0$ and $q_B = 100$ before the systems come in thermal contact. What is the probability of being in this state after the system has reached equilibrium?

Solution:
Calculated by the same program. The value is $1.4820 \cdot 10^{-19}$.

The microstate of the system is given by the energy of each oscillator given as n_i for each of the oscillators. We start by studying a single system with N oscillators and energy q. You can generate the initial state by placing each energy unit in a random oscillator. (Some oscillators may receive more than

one energy units and some may receive none). At each timestep we attempt a transfer of energy from one oscillator to another oscillator using the following algorithm. Select an oscillator n_1 at random. If the oscillator has zero energy, do nothing, if the oscillator has a positive energy, select another oscillator n_2 at random and transfer one unit of energy from n_1 to n_2. Repeat the process for as many "timesteps" as you want.

(p) Write a program to generate the initial microstate and the "time" development of the microstate. Plot the initial state and the state after 100 flips.

Solution:

```
% MC for a two part Einstein crystal
clear all;
NA = 100;
NB = 100;
qA = 300;
qB = 0;
q = qA + qB; % Total energy
N = NA + NB;
state = zeros(N,1);
% Generate initial, random state
placeA = randi(NA,qA,1);
for ip = 1:length(placeA);
    i = placeA(ip);
    state(i) = state(i) + 1;
end
placeB = randi(NB,qB,1);
for ip = 1:length(placeB);
    i = placeB(ip);
    state(i) = state(i) + 1;
end
plot(state)
% Simulate state development
nstep = 100000;
EA = zeros(nstep,1);
EB = EA;
for istep = 1:nstep
    % Select oscillator at random
    i1 = randi(N,1,1);
    % Check if it has energy
    if (state(i1)>0)
        % Then find other state
        i2 = randi(N,1,1);
        state(i2) = state(i2) + 1;
        state(i1) = state(i1) - 1;
    end
```

```
    % Plot
    subplot(2,1,1)
    plot(state),drawnow
    xlabel('i');
    ylabel('n_i');
    subplot(2,1,2); % Avg energy in each system
    EA(istep) = sum(state(1:NA))/NA;
    EB(istep) = sum(state(NA+1:end))/NB;
    plot((1:istep),EA(1:istep),'-r',(1:istep),EB(1:istep),'-
        b');
    drawnow
    xlabel('t');
    ylabel('q_A/N_A , q_B/N_B')
end
```
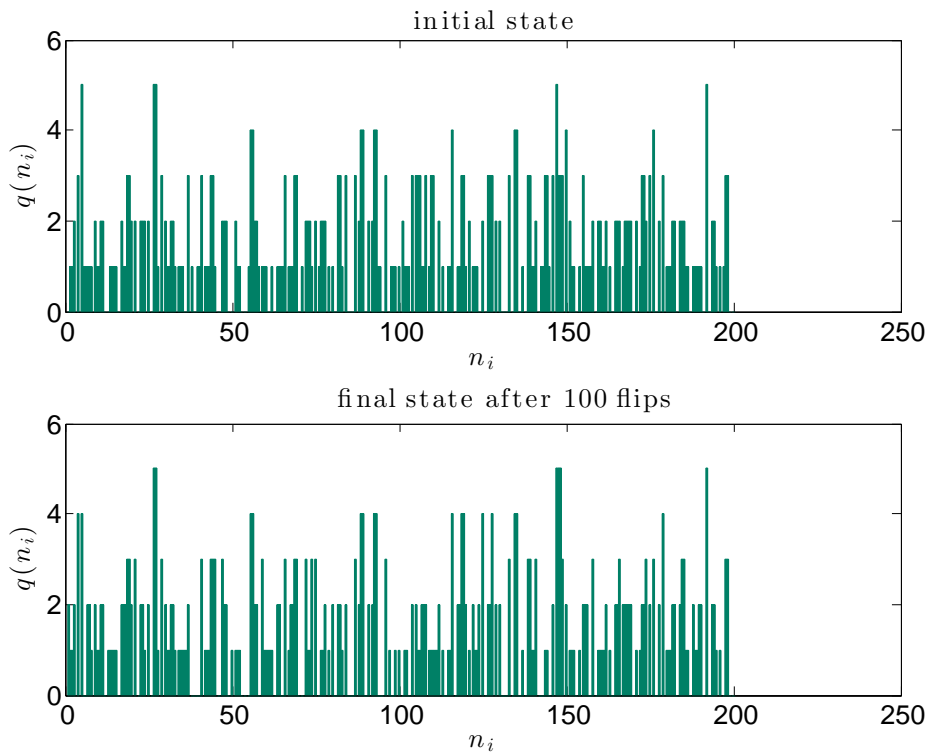

Figure 2: Plot of the initial and the final state after 100 flips. N=200, q=300.

(q) Divide your system into two parts, each part having $N/2$ oscillators. We call the first $N/2$ oscillators system A corresponding to oscillators $i = 1, N/2$, and the second $N/2$ oscillators system B, corresponding to oscillators $i =$

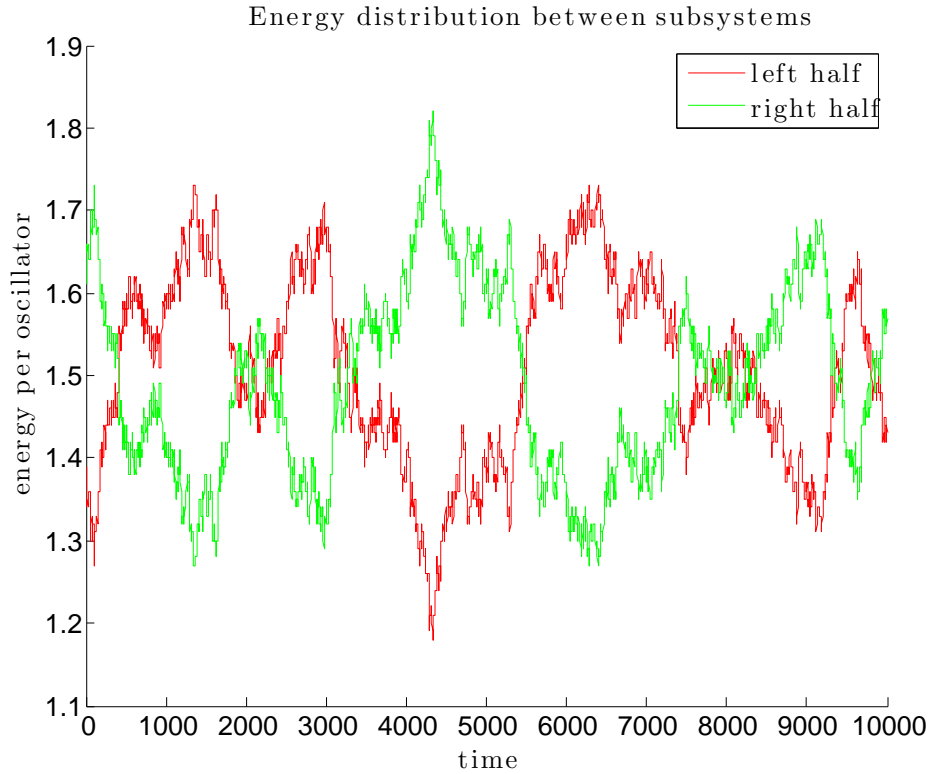$N/2 + 1, N$. Plot q_A/N_A and q_B/N_B as a function of time. Comment on the result.

Solution:

Figure 3: Time evolution of the energy distribution between the two subsystems. N=200, q=300.

(r) Initialize the system with all the energy in the system A only. Plot the average energy per oscillator (q_A/N_A and q_B/N_B) as a function of time and and comment on the result.

Solution:

(s) Starting from an equilibrium configuration (either by starting from a random configuration or by running a non-random configuration for a long time before starting measurements) plot the probability of the macrostates. Comment on the results.
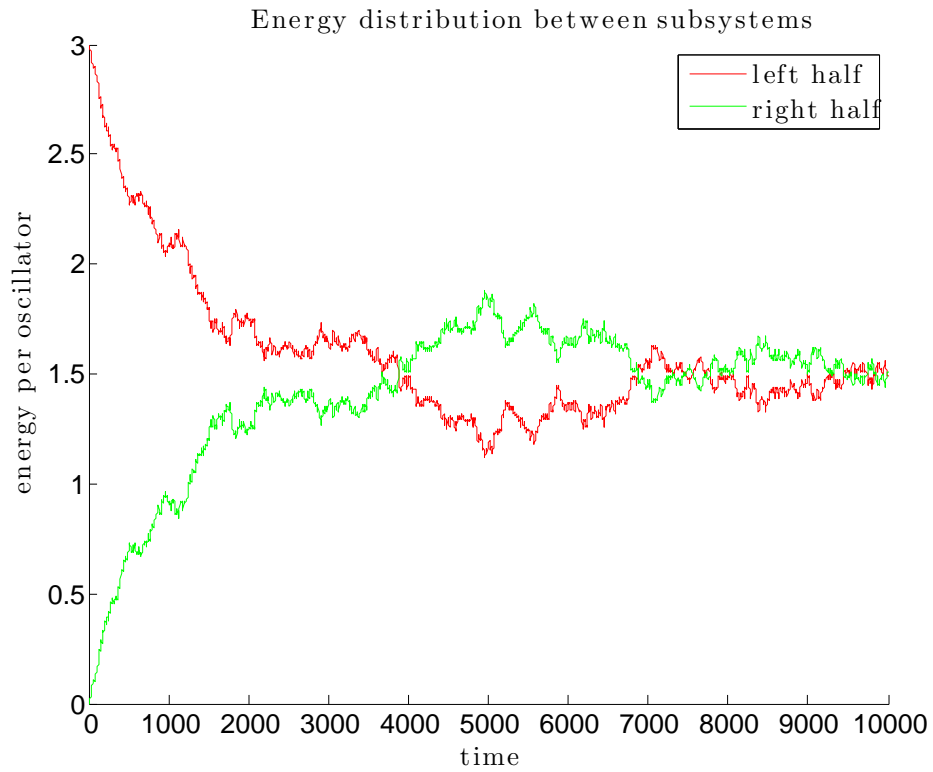
Figure 4: Time evolution of the energy distribution between the two subsystems. Initially all energy is in the left subsystem. N=200, q=300.
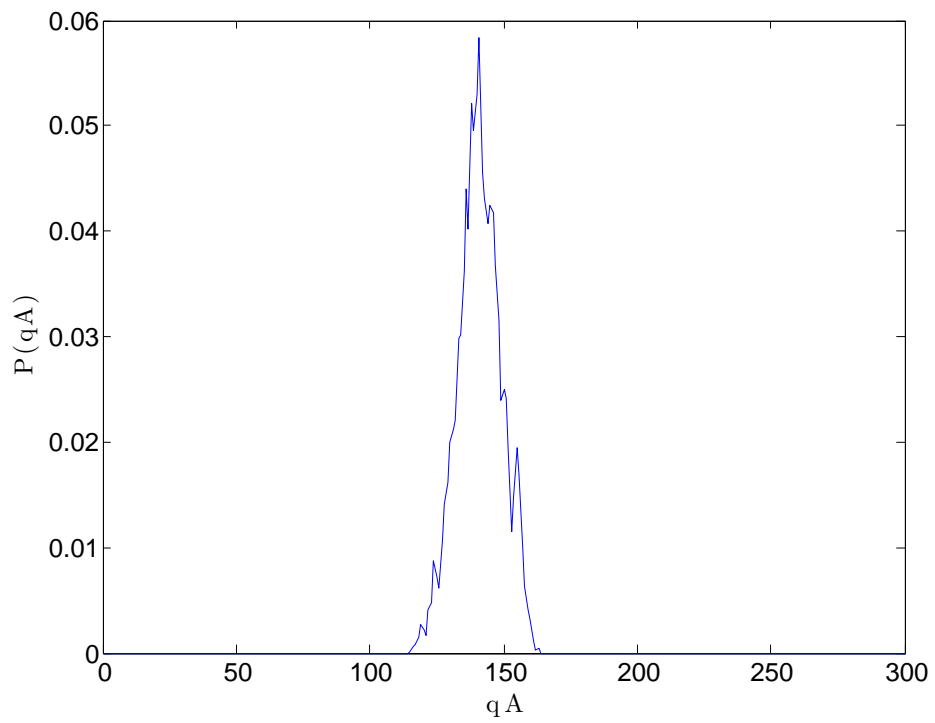
Solution:

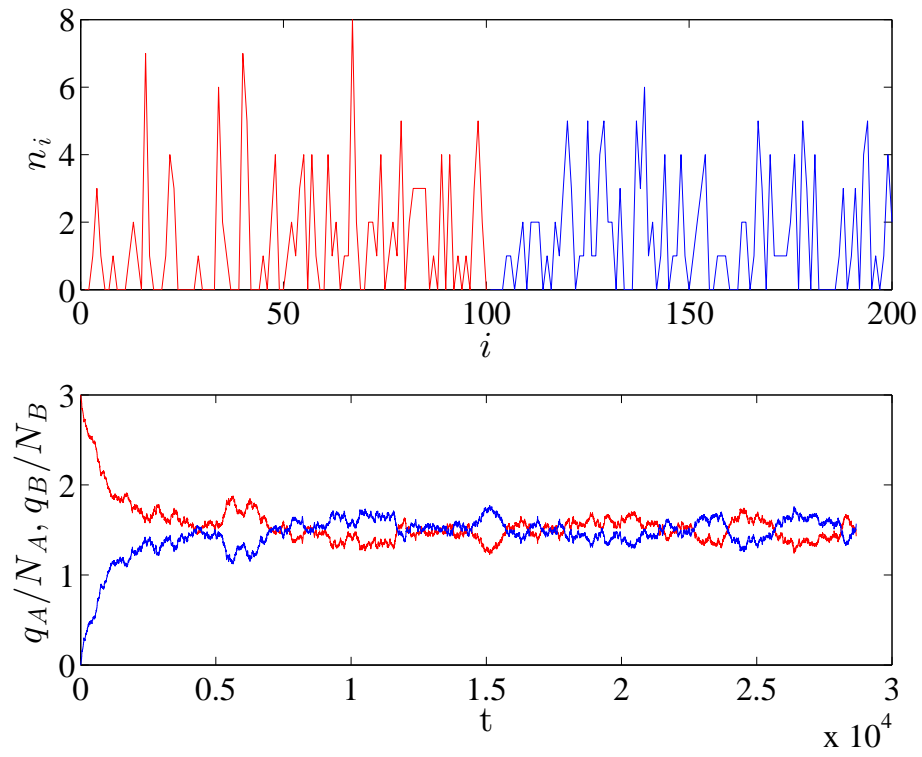Figure 5: Probability of the macrostates. N=200, q=300.

Figure 6: Example state (top) and time development of the average energy per oscillator for a system divided into two parts A and B.